Point and Spacegroup Issues

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1 Notation

A group is written with a calgraphic font ($\mathcal{G}$). Matrices and vectors are in bold ($\mathbf{R}, \mathbf{t}$). In the main text, a group denoted by the XXX-group is often used. The XXX group in this context is a group derived from the spacegroup, by removing all translational component dues to screw axis and glide plane, while keeping the translation due to the lattice. Furthermore, all rotation axis go through the origin. (**IT WOULD BE GOOD IF YOU CUOLD EXPLAIN ME HOW YOU EXACTLY DO THIS**). The group generated ni this manner, is similar to the point group of the lattice, albeit that the centering of the lattice is preserved.

2 Introduction

This brief set of notes describes a recent implementation of some space and point group related algorithms used for the automatic determination of space groups. The algorithms described here handle mainly with how candidate space groups are derived. For this, 3 different problems needed to be tackled. Each of these sub problems will be explained in a different section. It is the hope that this brief report could be transformed into a (at least) short communication. In the remainder of this report, the central problem will be identified and a possible solution will be proposed. Technical details follow in separate sections.

3 Problem statement

The problem this report deals with the generation of likely spacegroups given a candidate spacegroup and a lattice.Assumed is the following:

1. The crystal lattice is only approximately correct. Higher lattice symmetries with an obliquity up to $\omega_{\max}$ degrees are possible as well.

2. The systematic absenses dictated by the given spacegroup are correct. It is however not guaranteed that all systematic absenses have been identified.

Given these two boundary conditions, a procedure has been developed that allows the automatic generation of all spacegroups possible. The problem can be solved in two stages:

1. Find all groups that are a supergroup of the pointgroup of the assumed spacegroup and a subgroup of the symmetry of the lattice.

2. for each pointgroup group, find all possible space groups that do not violate the systematic absences condition imposed by the original spacegroup

The latter two subproblems can efficiently be tackled using the tools available in the CCTBX (XXX) and will be presented below. An associated problem to the ones mentioned above, is the ability to map the crystal symmetry to the reference setting. Althuogh the tools in the CCTBX allow a spacegroup to be transformed to its reference setting, no satisfactory tools were available to transform both space group and unit cell to the preferred setting.

4 The construction of a point group graph

For issues beyond the scope of this communication, it is essential that the exploration of possible pointgroups is caried out by reducing the the unit cell to the Niggli cell (XXXX). Given the Niggli cell, the symmetry of the lattice can be obtained using a prodecure developed by Le-Page, albeit modified using ideas published elsewhere and utilising some novel shortcuts based on the work Lebedev, Vagin & Murshudov. The point group of the assumed symmetry is denoted by $\mathcal{G}_0$. The pointgroup of the lattice is denoted by $\mathcal{G}_N$. Using the technique of coset decomposition, all unique symmetry elements $\{\mathbf{R}\}$ in $\mathcal{G}_N$ that are not present in $\mathcal{G}_0$ are found. The elements of $\{\mathbf{R}\}$ can be used to construct all minimal supergroups of the given point group $\mathcal{G}_j$ by multiplying in a single given element of $\{\mathbf{R}\}$ denoted by $\mathbf{R}_n$:

$$\mathcal{G}_k = \mathbf{R}_n \mathcal{G}_j \tag{1}$$

say something about the fact that only M minimal supergroups are generated, eventhough there are N symops. also, mention that if Rn generates Gk,

then Ro can be an element of Gk, eventhough Ro*Gj!=Gk. bladibla left over symops.

The relations between the groups and minimal supergroups generated in this way, can be stored in a graph, whose vertices represent point groups and who's edges represent a group, minimal supergroup relation. The edges can be assigned the set of symmetry elements that generate the minimal supergroup of $\mathcal{G}_j$. The above procedure can be iterated until no new groups are generated.

The obtained graph can be used in decision making processes involving the determination of the point group of a certain dataset. If for instance, a particular point group is found to be imcompatible with the experimental data, all possible supergoups of this particular point group can be eliminated as possible candidates.

4.1 Example

Given the unit cell $(30, 30, 50, 90, 90, 90)$ and an assigned point P2, it is easy to see that the lattice symmetry is P422. The point group graph is as follows

1. P121 $\rightarrow$ P222, using $(\bar{h}, \bar{k}, l)$
2. P121 $\rightarrow$ P422, using $(\bar{k}, \bar{h}, \bar{l}), (\bar{h}, \bar{k}, l), (k, h, \bar{l})$
3. P222 $\rightarrow$ P422, using $(\bar{k}, \bar{h}, \bar{l})$

Note that both P121 and P222 are maximal subgroups of P422. The grouping of symmetry elements in the graph allows one to quickly identify sets of symmetry operators that are linked together in a certain pointgroup transition. For instance, the application of $(k, h, \bar{l})$ on P121, generates point group P422, which contains the elements $(\bar{k}, \bar{h}, \bar{l})$ and $(\bar{h}, \bar{k}, l)$. These elements are thus linked together for this particular relation between point groups.

Also note that if for any reason point group P222 cannot be considered the 'true' pointgroup of the crystal, neither can P422 (P222 is a subgroup of P422). This type of reasoning might be usefull in quickly eliminating 'upstream' point groups.

5 Best cell determination

Given that the reader is familiar with the notion of a *spacegroup reference setting*, consider an associated concept named *best cell*, or maybe better *preferred setting*

of the crystal symmetry. Define the preferred setting of the crystal symmetry as that choice of unit cell and space group for which $a \leq b \leq c$ (or $a \leq b$ or $a \leq c$ in certain spacegroups) while the space group is in a reference setting at the same time. The crystal symmetry preferred setting can be found in the following manner. There are 6 change of basis operators that described a permutation of the axis:

1. $\mathbf{R}_1 = (x, y, z)$
2. $\mathbf{R}_2 = (-x, z, y)$
3. $\mathbf{R}_3 = (z, -y, x)$
4. $\mathbf{R}_4 = (y, x, -z)$
5. $\mathbf{R}_5 = (y, z, x)$
6. $\mathbf{R}_6 = (z, x, y)$

For a given space group in the reference setting$\mathcal{G}_{\mathrm{ref.set}}$, apply the change of basis operator:

$$\mathcal{G}_{\mathrm{axespermut}} = \mathbf{R}_j \mathcal{G}_{\mathrm{ref.set}} \mathbf{R}_j^{-1} \tag{2}$$

The now obtained spacegroup is not neccesarily in the reference setting, but has an associated operator, $(\mathbf{R}_{2\mathrm{ref}}, \mathbf{t}_{2\mathrm{ref}})$ to put the space group back to its reference setting. If the rotational part of the operator that bring the space group to its closets reference setting is equal to the identity operator (x, y, z) application of both the axes permutation and the change of basis to the reference setting results, in effect, in only a permuation of the axis, while the space group stays intact. This procedure can be carried out for each axes permuation while storing succesfull transformations. Note that if the permuations are visted in the order as written above, it is easy to determine if one of the axis is 'fixed':

1. If $\mathbf{R}_1$ is allowed permutation: fixed_axis=a
2. If $\mathbf{R}_1$ is allowed permutation: fixed_axis=b
3. If $\mathbf{R}_1$ is allowed permutation: fixed_axis=c
4. If $\mathbf{R}_1$ is allowed permutation: fixed_axis=$None$
5. If $\mathbf{R}_1$ is allowed permutation: fixed_axis=$None$

For each of the allowed axes permuations, one can now decide which order of cell constants is preferred.

6 Point group and systematic absense compatible space groups

I'll have a glass of wine now i guess.